Phase separation in fermionic systems with particle-hole asymmetry

Arianna Montorsi
Dipartimento di Fisica del Politecnico and CNISM,
corso Duca degli Abruzzi 24, I-10129, Torino, Italy
(Dated: March 12, 2008)

We determine the ground-state phase-diagram of a Hubbard Hamiltonian with correlated hopping, which is asymmetric under particle-hole transform. By lowering the repulsive Coulomb interaction U at appropriate filling and interaction parameters, the ground state separates into a hole and an electron conducting phases: two different wave vectors characterize the system and charge-charge correlations become incommensurate. By further decreasing U another transition occurs at which the hole conducting region becomes insulating, and conventional phase separation takes place. Finally, for negative U the whole system eventually becomes a paired insulator. It is speculated that such behavior could be at the origin of the incommensurate superconducting phase recently discovered in the 1D Hirsch model. The exact phase boundaries are calculated in one dimension.

PACS numbers: 05.30.Fk, 71.10.Fd

One very debated issue in the context of correlated fermionic materials is the occurrence of phase separation (PS). For instance, in ultracold fermionic atoms trapped on optical lattices PS appears when the superfluid phase coexists with the normal phase [1, 2]; these systems may be investigated by means of the negative U Hubbard model [3]. Also, in high-T_c materials PS leads to the formation of one-dimensional stripes[4]. It is believed that the phenomenon could be a consequence of the interplay between antiferromagnetic order and holes propagation; as such, its appearance is investigated within the context of the $t-J$ model [5, 6, 7, 8], which describes the Hubbard model in the limit of strong repulsive Coulomb interaction. In the present paper we suggest a further scenario for the occurrence of PS in Hubbard-like systems, resulting from competition between conducting phases with different charge: in the hole rich region the carriers are the electrons, while in the pair rich region they eventually become the holes. In absence of particle-hole symmetry, the proposed mechanism can generate incommensurability. The mechanism is proven to survive in dimension greater than 1 for a simple case.

We study the bond-charge extended Hubbard Hamiltonian, which has been introduced to describe compounds containing extended orbitals [9]. It comes from assuming that the charge in the bond affects the effective potential acting on valence electrons; the extension of the Wannier orbitals and the hopping between them should vary with the charge. A generalization of that Hamiltonian is the $U-X-X'$ Hamiltonian introduced in [10]. In the grand-canonical ensemble it reads:

$$H_{BC} = -\sum_{\sigma=\uparrow,\downarrow,\langle ij\rangle} [1 - x(n_{i-\sigma} + n_{j-\sigma}) + x' n_{i-\sigma} n_{j-\sigma}] (c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.}c.) + u \sum_i n_{i\uparrow} n_{i\downarrow} - \mu(\sum_{i\sigma} n_{i\sigma} - N) \quad ,$$

where the lower case symbols denote that the coefficients of the interactions have been normalized in units of the hopping amplitude, and the 3-body interaction term x' appears as an effective interaction from the three band-model. Moreover N is the number of electrons on the D-dimensional L sites lattice Λ_D. The model belongs to the class of Hubbard Hamiltonians with correlated hopping, which contains some integrable cases that have been widely studied in recent years (see [11] and references therein).

H_{BC} is in general is not invariant under particle-hole transform. For this reason the model has been first proposed (for $x' = 0$) in two dimensions, motivated by a theory of hole superconductivity [12]. It was investigated by means of bosonization approach in [13] at half-filling for arbitrary (and weak) x and x'. Also, a particle-hole invariant subcase of H_{BC}, which takes place at $x' = 2x$, has been previously discussed[14].

Recently, it has been proven [15],[16] that in 1D at half-filling H_{BC} displays a rich phase diagram already at $x' = 0$, quite different from that of the Hubbard model, and from that derived in the weak coupling limit [13]. In particular, at sufficiently low $u > 0$, and for appropriate range of x values an unexpected incommensurate superconducting (ICSS) phase appears, which drives the usual transition to an insulating state to higher values of u. Here we investigate the origin of such phase by constructing the exact ground-state phase-diagram of a

particular sub-case of (1) still asymmetric under particle-hole transform.

Hamiltonian (1) can be written in terms of the Hubbard projectors, $X_i^{\alpha\beta} \doteq |\alpha\rangle_i \langle\beta|_i$; here $|\alpha\rangle_i$ are the states allowed at a given site i, $\alpha = 0, \uparrow, \downarrow, 2$ ($|2\rangle \equiv |\uparrow\downarrow\rangle$). Inserting the choice $x = 1$ in H_{BC}, the resulting Hamiltonian $H \equiv H_{BC}(x = 1)$ turns out to preserve the number of doubly occupied states $N_d =< \hat{N}_d >\doteq< \sum_j X_j^{22} >$: $[H, \hat{N}_d] = 0$ for arbitrary x', D and N. In the following, we shall adopt such choice. H can then be written as

$$H = H_{01} + H_{12} - \mu(L - N) \quad ,$$

where

$$\begin{aligned} H_{01} &= -\sum_{\langle i,j\rangle\sigma} (X_i^{\sigma 0} X_j^{0\sigma} + h.c.) + \mu \sum_i X_i^{00} & (1) \\ H_{12} &= -t_x \sum_{\langle i,j\rangle\sigma} (X_i^{2\sigma} X_j^{\sigma 2} + h.c.) + (U - \mu) \sum_i X_i^{22} & (2) \end{aligned}$$

with $t_x = 1 - x'$. We shall limit our analysis to the range $0 \leq t_x \leq 1$. By implementing the transformation $c_{i,\sigma} \to c_{i,\sigma}^\dagger$, it can be realized that the range is representative of the behavior of the model at any t_x value. In the two limits $t_x = 0$ ($x' = 1$) and $t_x = 1$ ($x' = 0$) the Hamiltonian reduces to known cases, namely the infinite U Hubbard model, and the bond-charge Hubbard model at $x = 1$ [17], both integrable in one dimension.

On general grounds, we expect that at large enough positive u the ground state would contain the minimum number of doubly occupied sites. Hence it will coincide with that of the infinite U Hubbard model (no doubly occupied sites) for $N \leq L$, and with its particle-hole counterpart for $N \geq L$. In Fig. 1 such state is denoted as $U\infty$. Also, for large enough negative u, the number of doubly occupied sites will be maximized, so that for even number of electrons the hopping term will be ineffective and the ground state would be a highly degenerate insulator consisting of $N/2$ pairs of electrons. In Fig. 1 this is denoted as PI (paired insulator). In order to investigate what happens between these two limits, let us think of the Hilbert space as factorized into three orthogonal subspaces,

$$\mathcal{H} = \mathcal{H}_{01} \oplus \mathcal{H}_{12} \oplus \mathcal{H}_\perp \quad : \tag{3}$$

states with no doubly occupied sites belong to $\mathcal{H}_{01}$, states with no empty sites live in $\mathcal{H}_{12}$, and the remaining states stay in $\mathcal{H}_\perp$. H_{10} does not act on doubly occupied sites present in $\mathcal{H}_\perp$, and annihilates states belonging to $\mathcal{H}_{12}$; hence, at given N_d and N, it reaches its minimum in $\mathcal{H}_{01}$. Analogously, H_{12} does not act on empty sites present in $\mathcal{H}_\perp$, and annihilates states in $\mathcal{H}_{01}$, hence reaching its minimum in $\mathcal{H}_{12}$. So that, at any given N and N_d, the absolute minima of both H_{10} and H_{12} (and consequently of H) are reached in the space orthogonal to $\mathcal{H}_\perp$. We can then rewrite the ground state energy E_{gs} in the form

$$E_{gs} = min_{|\psi\rangle\in\mathcal{H}} \langle\psi|H|\psi\rangle \equiv min_{|\psi\rangle\in\mathcal{H}_{01}\oplus\mathcal{H}_{12}} \langle\psi|H|\psi\rangle \quad , \tag{4}$$

where the minimum has to be taken with respect to N_d, the constraint $L - N = N_e - N_d$ is implemented through the chemical potential, and $N_e \doteq \sum_i X_i^{00}$ is the (conserved) number of empty sites. More explicitly, one could look for a ground state of the form:

$$|\psi(N_e, N_d)\rangle_{gs} = a|\psi_{01}(N_e')\rangle + \sqrt{1 - a^2}|\psi_{12}(N_d')\rangle \quad , \tag{5}$$

where a is a further variational parameter, and $N_e = a^2 N_e'$, $N_d = (1 - a^2) N_d'$. Here $|\psi_{01}(N_e')\rangle \in \mathcal{H}_{01}$, and $|\psi_{12}(N_d')\rangle \in \mathcal{H}_{12}$ are the ground states of H_{01} at given N_e' and H_{12} at given N_d' respectively. The corresponding energies are recovered from those of the infinite U Hubbard model, E_{gs}^∞. In fact, the spectra of H_{01} and H_{12} are the same: up to a multiplicative factor t_x, and to the conserved quantities N_e, N_d, they coincide with the spectrum of the infinite U Hubbard model. Explicitly,

$$\begin{aligned} E_{gs} &= a^2 E_{gs}^\infty(N_e') + (1 - a^2)\left[t_x E_{gs}^\infty(N_d') + u N_d'\right] \\ &- \mu\left(N_d - N_e + L - N\right) \quad . \end{aligned} \tag{6}$$

By minimization of E_{gs} with respect to μ one obtains that the actual value of a^2 is given by

$$a^2 = \frac{L - N + N_d'}{N_e' + N_d'} \quad . \tag{7}$$

The case $a^2 = 1$ ($a^2 = 0$) correspond to the $U\infty$ phase described above for $N \leq L$ ($N \geq L$), with $N_e' = L - N$ ($N_d' = N - L$). Apart from these limits, the system is always separated into two phases, characterized by N_e', N_d', and μ values which minimize E_{gs} as given by (6), at given t_x and u. Such values do not depend on the actual filling N: PS implies that the chemical potential is constant with the filling.

Since $t_x \leq 1$, independently of the actual value of E_{gs}^∞ (and D) one could expect three different behavior to emerge from the minimization equations within the PS phase, depending on the filling and the interaction parameters.

(i) $N_e' < N_d' < L$: both the coexisting phases are conducting. They are characterized by different Fermi momenta $k_F^{(e)}$ and $k_F^{(d)}$, which can be inferred from those of the corresponding infinite U model, and are in general not commensurate between each other. For this reason we characterized the phase as IPS, incommensurate phase separation. Later on we shall discuss how such incommensurability reflects onto some physical feature.

(ii) $N_e' < N_d' = L$; only the hole-rich region is conducting, whereas the other phase is a paired insulator.

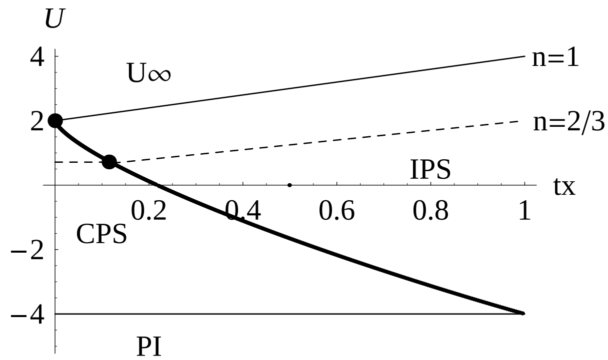

Figure 1: (Color online) Phase diagram in the u-t_x plane in $D = 1$: the transition to the $U\infty$ region depends on the filling n, whereas the other transitions are independent of it. CPS and IPS denote the conventional and the incommensurate phase separation regions respectively; PI stays for paired insulator. Full dots indicate the tricritical points.

The system is characterized by the Fermi momentum $k_F^{(e)}$ of the conducting electrons, *i.e.* that of the infinite U Hubbard model at a filling $L - N'_e < N$. We denote such phase as CPS (conventional phase separation).

(iii) $N'_e = N'_d = L$; both phases are insulating. In this case we are in one of the infinitely many (in the thermodynamic limit) degenerate ground states characterizing the PI phase.

A further interesting limiting case, not discussed above though contained in the minimization equations, occurs when $N'_e = N'_d \neq L$. In such case both phases are conducting as in (i), but they are characterized by the same Fermi momentum, $k_F^{(e)} = k_F^{(d)}$. This is the case for $t_x = 1$. The latter is the already mentioned bond-charge Hubbard model at $x = 1$ [17], and manifests particle-hole invariance. This example illustrates how in our scheme the IPS phase, intended as the appearance of two not commensurate modulations, is in fact associated with the presence of particle-hole asymmetry.

In order to make the above predictions more quantitative, we now turn to the discussion of the 1D case. In that case the ground-state energy per-site of the infinite u Hubbard model is known exactly. In the thermodynamic limit it reads:

$$E_{gs}^{\infty}(n) = -\frac{2}{\pi}\sin(\pi n) \quad , \tag{8}$$

with n average per-site filling, $n \doteq \frac{N}{L}$.
When inserted into E_{gs}/L, as given by (6), the above information allows for an explicit derivation of the ground-state phase diagram, shown in Fig. 1. This is achieved by solving the minimization equations with respect to $n'_e \doteq \frac{N'_e}{L}$ and $n'_d \doteq \frac{N'_d}{L}$, which in turn fix $k_F^{(e)} = \pi(1 - n'_e)$ and $k_F^{(d)} = \pi(1 - n'_d)$.
Interestingly, the same phase diagram and ground-state energy can be also obtained by generalizing the approach developed in [18] for studying PS in the extended Hubbard model for $V \to \infty$, with V neighboring sites diagonal Coulomb interaction. At a given filling, the ground state can be thought of as an island of $N_d + Z$ singly and doubly occupied sites inserted into a chain of $L - N_d - Z$ singly and empty sites. Such choice allows to maximize the number of available low energy momenta. In the thermodynamic limit, minimizing the energy of that state with respect to N_d and Z gives precisely the same phase diagram obtained here in Fig. 1. It turns out that the following relations hold: $n'_d = \frac{N_d}{N_d + Z}$, and $n'_e = \frac{L - N + N_d}{L - N_d + Z}$.

The solutions $n'_e = 1 - n$ ($a^2 = 1$) below half-filling, and $n'_d = 1$ ($a^2 = 0$) above half-filling, are obtained for $u > u_c(n, t_x)$ (see below). These identify the $U\infty$ phase. In particular, at $n = 1$ a charge gap Δ_c opens and the phase becomes insulating: for $u \geq u_c(1, t_x) = 2(t_x + 1)$, $\Delta_c = u - u_c$.
For $a^2 \neq 0, 1$ the solution to the minimization equation reads:

$$n'_e = \frac{1}{\pi}\arccos\left(\frac{\mu}{2}\right) \ , \ n'_d = \begin{cases} \frac{1}{\pi}\arccos\left(\frac{u-\mu}{2t_x}\right) & \text{IPS} \\ 1 & \text{CPS} \end{cases} . \tag{9}$$

Minimizing E_{gs} is thus reduced to solving the following transcendental equation in μ,

$$\mu = \frac{1}{n'_e + n'_d}\left(-2t_x \sin \pi n'_d + u n'_d + 2 \sin \pi n'_e\right) \quad , \tag{10}$$

with n'_e and n'_d as specified in (9). Let us denote the solution by $\bar{\mu}(u, t_x)$. The actual value of $\bar{\mu}_I$ in the IPS phases is limited by the constraint

$$\bar{\mu}_I \in \,]\max(-2, u - 2t_x), \min(2, u + 2t_x)[\quad . \tag{11}$$

Whereas in the CPS phase μ becomes independent of t_x, and $\bar{\mu}_C(u)$ is the solution of (10) for $n'_d = 1$. In fact, all the transition curves can be characterized by the value of $\bar{\mu}$ along them:

1. $U\infty \to IPS, CPS$,

$$\bar{\mu}(u, t_x) = \begin{cases} -2\cos(\pi n) & n \leq 1 \\ u + 2t_x \cos(\pi n) & n \geq 1 \end{cases} \tag{12}$$

2. $IPS \to CPS$, $\bar{\mu}_I = \bar{\mu}_C$; the transition occurs at $\bar{t}_x = [\bar{\mu}_C(u) - u]/2$, implying $n'_d = 1$.

3. finally at $CPS \to PI$ $\bar{\mu}_C = -2$.

When passing from μ to n, one realizes that only the two transitions 1 do depend on the filling, whereas the others are independent of it. At transition 1 the explicit value of $u_c(n, t_x)$, is obtained by solving eq. (12) for u. Transition 2 takes place at $t_x = \bar{t}_x$; transition

3 occurs at $u = -4$. As an example, we report the critical curves in fig. 1 in the (u, t_x) plane at two different filling values. For $u \leq 2$, depending on n, two tricritical point (T1) are recognized, characterized by the merging of $U\infty$, IPS and CPS phases: one (not shown) occurs at $n = 2$, whereas the other one occurs at the same u value and at a filling $n_{T1} \leq 1$. Analytical calculations show that $u_{T1} = -2(\cos[\pi n_{T1}] + t_x)$, $n_{T1} \approx \frac{1}{\pi}\arccos[(3t_x - 1)/(1 + t_x)]$. Increasing t_x progressively drives the system to a particle-hole symmetric diagram. For $t_x = 1$ $n_{T1} = 0$, which is the particle-hole counterpart of the tricritical point in $n = 2$. The critical curves in the (u,n) plane (not shown) highlight that particle-hole asymmetry ($t_x \neq 1$) favors the IPS phase at filling greater than half, in which case it survives at appropriate positive u values up to $n = 2$. Fig. 1 also shows that the infinite U Hubbard model ($t_x = 0$) exhibits CPS for $u \leq 2$ if doubly occupied sites are allowed.

In order to clarify the meaning of the different modulations in the IPS phase, we also give in Fig. 2 the charge-charge correlations $C(r) \doteq \langle (n_i - n)(n_{i+r} - n)\rangle$ at half filling (upper part), and their Fourier transform $N(q) \doteq \sum_r e^{iqr} C(r)$ (lower part). Since $C(r)$ can be evaluated exactly (see for instance [19]), we can also provide an analytic expression for $N(q)$, which reads:

$$N(q) = C(0) + (\delta(q) - 1)d_{PS} - a^2\gamma_{k_F^{(e)}}(q) - (1 - a^2)\gamma_{k_F^{(d)}}(q) \quad . \tag{13}$$

Here $\delta(q)$ is the Dirac delta, and $d_{PS} = (1 - n + n'_d)(n - 1 + n'_e)$ is the constant responsible for the divergent contribution in $q = 0$ characteristic of phase separation: at given (u, t_x) it becomes zero for $n < n_l \doteq 1 - n'_e$, or $n > n_h \doteq 1 + n'_d$. Moreover

$$\gamma_k(q) = -\frac{1}{4\pi^2}\mathcal{R}[L_2(e^{i(q+2k)}) + L_2(e^{i(q-2k)}) - 2L_2(e^{iq})] \quad , \tag{14}$$

with $k = k_F^{(e)}, k_F^{(d)}$, and $L_2(z)$ denoting the dilogarithm of z (R[] being the real part of []), describes the q-dependence of density correlations. Equations (13)–(14) enlighten how in the IPS phase two wave-vectors do characterize $N(q)$, namely $q^{(e)} = 2k_F^{(e)}$ and $q^{(d)} = 2k_F^{(d)}$, as shown in the lower part of Fig. 2. Whereas in the CPS phase, since $k_F^{(d)} = 0$ and $\gamma_0(q) = 0$, only one feature characterizes $N(q)$, namely the wave-vector of the single fermion problem corresponding to a filling $n = 1 - n'_e$. It can be recognized that the above type of ground-state phase diagram could explain different features displayed by the non-integrable 1D Hirsch model discussed in [16]. At variance with the present model, in that case the model still had arbitrary t_x ($t_x = 2x - 1$) but also $x' = 0$, implying the appearance of a further term in the Hamiltonian. The numerical solution did show incommensurate charge-charge correlations (and superconductivity) at appropriate values of u and t_x, always missing particle-hole invariance. Also, by suitably varying u and t_x at half-filling, the system could first pass from an insulating phase, characterized by flat density correlations, to a conducting phase in which that correlations acquire a modulation; then to the ICSS phase in which further modulations occur. We suggest that the two latter phases could be identified with our CPS and IPS phases respectively. As an example, in fig. 2 we report $C(r)$ at u and t_x values identical with those used for the Hirsch model in fig. 3 of [16]. The resemblance of the two figures is convincing.

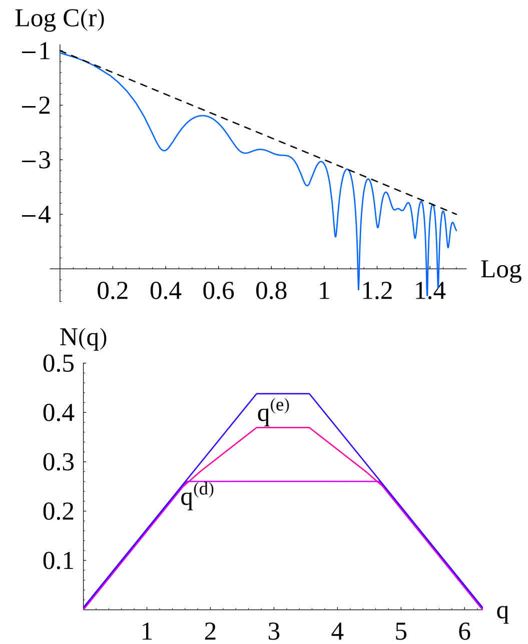

Figure 2: (Color online) (a) Equal time density correlations $C(r)$ vs distance r at $u = 1$ and $t_x = 0.6$; the dashed line represents the slope $1/r^2$. (b) $N(q) - d_{PS}$ at $t_x = .3$, $u = 0$, and three different fillings: from top to bottom $n = .5$ (blue), $n = 1$ (pink), $n = 1.7$ (violet).

In this paper, we have shown how the appearance of incommensurate characteristic wave-vectors in strongly interacting fermionic systems could be related to the occurrence of phase separation, in case the system is not symmetric under particle-hole transform. Recently the occurrence of incommensurate modulations in charge correlations was observed also in a Hubbard-like model including next-nearest neighbors hopping[20]. Since that model is particle-hole asymmetric, we suggest that IPS could occur in that case.
The mechanism could also be a natural candidate for explaining PS in unbalanced mixtures of cold fermionic atoms[1, 2]. In this case the PI phase should be interpreted as the (unpolarized) superfluid phase, and the CPS phase should be identified with coexistence of the superfluid with the (polarized) Fermi gas.

The author acknowledges useful discussions with A. Anfossi, C. Degli Esposti Boschi, A. Andreev, B. Spivak;

and the kind hospitality of the Department of Physics of the University of Washington for four months, during which this work was completed.

[1] M.M. Parish et al., Nature Phys. 3, 124 (2007).
[2] S. Pilati, S. Giorgini, Phys. Rev. Lett. **100** 030401 (2008)
[3] G. Xiaolong et al., Phys. Rev. Lett. **98**, 030404 (2007)
[4] J.M. Tranquada et al., Nature **375**, 361 (1995)
[5] V.J. Emery, S.A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990)
[6] W.O. Putikka, M.U. Luchini, and T.M. Rice, Phys. Rev. Lett. 68, 538 (1992)
[7] C. S. Hellberg, and E. Manousakis, Phys. Rev. Lett. **78**, 4609 (1997)
[8] M. Calandra, F. Becca, and S. Sorella, Phys. Rev. Lett. **81**, 5185 (1998)
[9] J. T. Gammel and D. K. Campbell, Phys. Rev. B **60**, 71 (1988); Y. Z. Zhang, *ibid* **92**, 246404 (2004);
[10] M.A. Simon, and A.A. Aligia, Phys. Rev. B 53, 15327 (1996)
[11] F.H. Essler, V. Korepin, and K. Schoutens, Phys. Rev. Lett. **68**, 2960 (1992); Phys. Rev. Lett. **70**, 73 (1993); R.Z. Bariev et al., J Phys A **26**, 1249 (1993); A. Montorsi, D.K. Campbell, Phys. Rev. B **53**, 5153 (1998)
[12] J. E. Hirsch, Physica C **158** 326 (1989); J. E. Hirsch and F. Marsiglio, Phys. Rev. B **39**, 11515 (1989).
[13] G.I. Japaridze, and A.P. Kampf, Phys. Rev. B 59, 12822 - 12829 (1999)
[14] M. Nakamura, K. Itoh, N. Muramoto, J. Phys. Soc. Jpn. 70, 3606 (2001); see also M. Nakamura, T. Okano and K. Itoh, Phys. Rev. B 72, 115121 (2005)
[15] A. Anfossi, C. Degli Esposti Boschi, A. Montorsi, and F. Ortolani, Phys. Rev. B **73**, 085113 (2006).
[16] A. Aligia *et al.*, Phys. Rev. Lett. **99**, 206401 (2007)
[17] L. Arrachea and A. A. Aligia, Phys. Rev. Lett. **73**, 2240 (1994); J. de Boer, V. E. Korepin, and A. Schadschneider, *ibid* **74**, 789 (1995).
[18] K. Penc, and F. Mila, Phys. Rev B **49**, 9670 (1994).
[19] A. Schadschneider, Phys. Rev. B **51**, 10386 (1995); A. Anfossi, P. Giorda, and A. Montorsi, Phys. Rev. B **75**, 1 (2007).
[20] G. I. Japaridze, R. M. Noack, and D. Baeriswyl, Phys. Rev. B **76**, 115118 (2007).